Spectral Statistics in Large Shell Model Calculations [1]

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Abstract

The spectral statistics of low–lying states of fp shell nuclei are studied by performing large shell–model calculations with a realistic nuclear interaction. For Ca isotopes, we find deviations from the predictions of the random–matrix theory which suggest that some spherical nuclei are not as chaotic in nature as the conventional view assumes.

1. Introduction

In recent years many authors have shown great interest in the fluctuation properties of energy levels[1)]. It is well known that the fluctuation properties of quantum systems with underlying classical chaotic behaviour and time–reversal symmetry agree

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with the predictions of the Gaussian Orthogonal Ensemble (GOE) of the random–matrix theory, whereas quantum analogs of classically integrable systems display the characteristics of the Poisson statistic[2].

In atomic nuclei, the fluctuation properties of energy levels are best studied in the domain of neutron and proton resonances near the nucleon emission threshold, where a large number of levels of the same spin and parity in the same nucleus are present, and an excellent agreement with GOE predictions has been found[3]. In the ground–state region, however, the samples of consecutive experimental levels of the same spin and parity in any one nucleus are quite small. Therefore it is more difficult to calculate reliable mean values and fluctuations of statistics such as energy level spacings. In order to circumvent this difficulty, in recent years[4,5,6] statistical analyses of experimental lower excitation energies have combined data from a large range of excitation energies and angular momenta of a nucleus or a set of nuclei. Such analyses have provided evidence suggesting that spherical nuclei show level spectra close to GOE predictions and deformed nuclei show strong deviations from GOE behaviour. In a recent analysis[7] of level spacings close to the yrast line of deformed nuclei with $Z = 62$–75 and $A = 155$–185, the average level spacing for states with the same spin and parity was calculated for the total ensemble instead of for individual nuclei. The level spacing fluctuations obtained are quite close to the Poisson distribution, showing evidence of regular motion.

We can conclude that experimental nuclear spectra suggest a dominance of chaotic motion in most cases and that regular motion seems to be prevalent in a small region of excitation energy just above the yrast line of deformed nuclei. But the borderlines in mass number, excitation energy, etc., between order and chaos in nuclei are not sharply distinguished by the experimental data available.

2. Analysis of the fp shell

Theoretical models should also help to establish the domains of chaos in nuclei. First of all, the success of the nuclear shell model and the collective models of nuclear structure at low excitation energies provide strong evidence of regular motion in nuclei. Theoretical studies of deformed nuclei have shown that a two–body interaction of reasonable strength causes chaotic spectra a few hundred keV above the yrast line due to rotational band mixing[8]. The transition from order to chaos has also been studied in the framework of the Interacting Boson Model and was found to depend on the values of the model parameters. Regular features of the spectra were found to be associated with values of the parameters for which the hamiltonian displays a symmetry[9]. However, statistical analyses of shell model energy spectra and wave functions have almost always shown that chaos in nuclei is quite widespread[10].

It is somewhat surprising that shell model calculations suggest such a prevalence of chaos because the model itself is based on a mean field idea associated with regular motion. The residual interaction can destroy the regularity of single–particle orbits

and cause the chaotic features, but it is still remarkable that chaos can be so dominant even for the lowest energy levels of light nuclei[11]. Recent shell–model calculations by Bae et al.[12] have shown that for nuclei of mass $A = 212$ shell model spectra display features of regular motion in some cases. The main reason for this seems to be the relatively small values of the residual interaction matrix elements as compared to the average spacing between neighbouring single–particle levels in heavy nuclei.

Table 1: m–scheme and maximal (J,T) dimensions of the analyzed configurations (n,p) of active nucleons.

	^{46}V	^{46}Ti	^{46}Sc	^{46}Ca	^{48}Ca	^{50}Ca
(n,p)	(3,3)	(4,2)	(5,1)	(6,0)	(8,0)	(10,0)
m–scheme dimension	121 440	86 810	30 042	3 952	12 002	17 276
(J,T)	$(4,0)$	$(4,1)$	$(4,2)$	$(4,3)$	(4,4)	(4,5)
(J,T) dimension	4 750	8 026	3 783	615	1 755	2 468

In this work, we undertake the statistical analysis of the shell–model energy levels in the $A = 46$–50 region. Exact calculations are performed in the ($p_{1/2}$,$p_{3/2}$,$f_{5/2}$,$f_{7/2}$) shell–model space, assuming a ^{40}Ca inert core. The diagonalizations are performed in the *m–scheme* using a fast implementation of the Lanczos algorithm through the code ANTOINE[14]. The interaction we use is a minimally modified Kuo–Brown force, explained in[15]. For a fixed number of valence protons and neutrons we calculate the energy spectrum for projected total angular momentum J and total isospin T.

Table 2: Number of energy levels up to 4 and 5 MeV above the yrast line in ^{46}V.

J	4 MeV	5 MeV
0	1	2
1	7	11
2	5	8
3	14	23
4	7	11
5	13	23
6	8	13
7	18	33
8	9	14
9	14	21
0–9	96	159

We calculate the $T = T_z$ states from $J = 0$ to $J = 9$ for all the combinations (n,p) of 6 active nucleons, i.e. (3,3), (4,2), (5,1) and (6,0). For the sake of completeness

we also calculated (8,0) and (10,0). Table 1 shows the m–scheme and the maximal (J,T) dimensions of the configurations (n, p) of active nucleons analyzed.

Since we are looking for deviations from chaotic features, we are mainly interested in the low–lying levels, up to a few MeV above the JT yrast line. Table 2 shows the number of levels up to 4 and 5 MeV above the yrast line in ^{46}V. As can be seen, in many cases the number of levels is too small to calculate fluctuations around the average spacing between neighbouring levels.

Hence in those cases we use a larger set of levels for the calculation of the mean level spacing as a function of energy. For each JT set of levels the spectrum is mapped into unfolded levels with quasi–uniform level density by using the constant temperature formula[5]. Under the 8 MeV range of energies the mean level density can be assumed to be of the form

$$\bar{\rho}(E) = \frac{1}{T} \exp\left[(E - E_0)/T\right], \tag{1}$$

where T and E_0 are constants. For fitting purposes it is better to use not $\bar{\rho}(E)$ but its integral $\bar{N}(E)$. We take

$$\bar{N}(E) = \int_0^E \bar{\rho}(E')dE' + N_0 = \exp\left[(E - E_0)/T\right] - \exp\left[-E_0/T\right] + N_0. \tag{2}$$

The constant N_0 represents the number of levels with energies less than zero. Following Shriner et al.[5], we consider Eq. 2 as an empirical function to fit the data and let N_0 take non–zero values. The parameters T, E_0 and N_0 that best fit $N(E)$ are obtained by minimizing the function:

$$G(T, E_0, N_0) = \int_{E_{min}}^{E_{max}} [N(E) - \bar{N}(E)]^2 dE, \tag{3}$$

where $N(E)$ is the number of levels with energies less than or equal to E. The energies E_{min} and E_{max} are taken as the first and last energies of the level sequence. As an example, Fig. 1 illustrates the fit to the integrated level density $N(E)$ for the $J^\pi T = 6^+1$ levels of ^{46}Ti.

Once the best fit $F(E)$ to $N(E)$ is obtained, the unfolded energy levels are given by

$$\tilde{E}_i = E_{min} + \frac{F(E_i) - F(E_{min})}{F(E_{max}) - F(E_{min})}(E_{max} - E_{min}). \tag{4}$$

These transformed energies should now display on average a constant level density ρ_c.

The spectral statistic $P(s)$ is used to study the local fluctuations of the energy levels[16,17]. $P(s)$ is the distribution of nearest–neighbour spacings $s_i = (\tilde{E}_{i+1} - \tilde{E}_i)\rho_c$ of the unfolded levels $\tilde{E}_i$. It is obtained by accumulating the number of spacings that lie within the bin $(s, s + \Delta s)$ and then normalizing $P(s)$ to unity.

For quantum systems whose classical analogs are integrable, $P(s)$ is expected to follow the Poisson limit, i.e. $P(s) = \exp(-s)$. On the other hand, quantal

Figure 1: The best fit to the integrated level density for ^{46}Ti with $J = 6^+$ and isospin $T - T_z = 0$.

analogs of chaotic systems exhibit the spectral properties of GOE with $P(s) = (\pi/2)s \exp(-\frac{\pi}{4}s^2)$ [1,2].

The $P(s)$ distribution is compared to the Brody distribution[18]

$$P(s,\omega) = \alpha(\omega+1)s^{\omega} \exp(-\alpha s^{\omega+1}), \tag{5}$$

with

$$\alpha = (\Gamma[\frac{\omega+2}{\omega+1}])^{\omega+1}. \tag{6}$$

This distribution interpolates between the Poisson distribution ($\omega = 0$) of integrable systems and the GOE distribution ($\omega = 1$) of chaotic ones.

In order to obtain a meaningful statistic, $P(s)$ is calculated using the unfolded level spacings of the whole set of $J = 0$–9 levels for fixed T up to a given energy limit above the yrast line. Thus the number of spacings included is reasonably large. For example, up to 4 MeV there are 52 spacings for $T = 0$ and 86 for $T = 1$, and up to 5 MeV there are 87 and 149 spacings, respectively. Table 3 shows the Brody parameter ω for the $J = 0$–9 set of level spacings for the $A = 46$ nuclei up to 4 and 5 MeV above the yrast line.

Clearly, ^{46}V and ^{46}Ti are highy chaotic, but there is a considerable deviation from GOE predictions in ^{46}Ca, which is a single closed shell nucleus. Similar calculations for ^{48}Ca and ^{50}Ca yield ω values similar to ^{46}Ca, as shown in Table 3. Thus, for

Figure 2: $P(s)$ for low–lying levels of the fp shell with $0 \leq J \leq 9$ for (n, p) configurations: $(3, 3)$ and $(4, 2)$. The dotted, dashed and solid curves stand for GOE, Poisson, and Brody distributions, respectively.

the Ca isotopes we find the same kind of phenomenon obtained by Bae et al.[12] in the heavy single closed nuclei ^{212}Rn and ^{212}Pb, namely that low–lying states deviate strongly from chaoticity toward regularity.

Table 3: Brody parameter ω for the fp shell for different configurations (n,p) of active nucleons with $0 \leq J \leq 9$ and $E \leq 4$ MeV (up) and $E \leq 5$ MeV (down).

^{46}V	^{46}Ti	^{46}Sc	^{46}Ca	^{48}Ca	^{50}Ca
0.97	1.09	0.65	0.57	0.64	0.56
0.97	0.97	0.93	0.57	0.50	0.65

To obtain a better estimate of the Brody parameter, we can separately combine spacings of different nuclei. In fig. 2 we plot $P(s)$ for the 236 spacings of ^{46}V+^{46}Ti, and in Fig. 3 for the 266 spacings of ^{46}Ca+^{48}Ca+^{50}Ca up to 5 MeV above the yrast lines. The number of level spacings is now sufficiently large to yield meaningful statistics and we see that Ca isotopes are not very chaotic at low energy, in contrast to other nuclei in the same region.

How may these results be explained? We observe that the two–body matrix el-

Figure 3: $P(s)$ for low–lying levels of the fp shell with $0 \leq J \leq 9$ for (n, p) configurations: $(6, 0)$, $(8, 0)$ and $(10, 0)$. The dotted, dashed and solid curves stand for GOE, Poisson, and Brody distributions, respectively.

ements of the proton–neutron interaction are, on average, larger than those of the proton–proton and neutron–neutron interactions. Consequently the single–particle motion in nuclei with both protons and neutrons in the valence orbits suffers more disturbance and is thus more chaotic. The shift towards the Poisson distribution obtained for the Ca isotopes could also be due to some underlying symmetry dominating the dynamics of those nuclei. However, we do not find significant differences between $J = 0$ and high J values when they are analyzed separately. Thus the seniority scheme does not seem to have a significant influence on the shift towards regularity observed in Ca isotopes.

It should be noted that the analysis[19] of experimental energy levels below 4.3 MeV excitation energy in the semi–magic nucleus ^{116}Sn yields a near–neighbour spacing distribution which is intermediate between GOE and Poisson, with $\omega = 0.51 \pm 0.19$. This result is consistent with the theoretical findings of Bae et al.[12] for ^{212}Rn and ^{212}Pb, and our present results for Ca isotopes.

3. Conclusions

Why do all shell model calculations give chaotic features for sd shell nuclei, without any significant deviations towards regularity? First, it should be noted that most

of these calculations include a large number of states, up to excitation energies far above the nucleon emission threshold. This is, for example, the case of the ^{22}O calculations of Bae et al.[12)], which include the full set of levels for several J values and obtain $\omega = 0.96$. Second, we notice that Ormand and Broglia[11)] obtained a GOE–like distribution for the first two spacings of each spectrum for a set of *sd* shell nuclei. However, these nuclei have valence protons and neutrons and are thus similar to the case of ^{46}V and ^{46}Ti, for which we also find chaotic behaviour. We conclude that no regular features have been found in the *sd* shell region. This is because single–closed nuclei have a small configuration space and too few low–lying levels for statistical analysis, and also because the disturbance of single–particle motion by the two–body interaction is greatest in light nuclei.

References

1. O. Bohigas, M. J. Giannoni, and C. Schmit, in *Quantum Chaos and Statistical Nuclear Physics*, Ed. T. H. Seligman and H. Nishioka (Springer–Verlag, Berlin, 1986); O. Bohigas and H. A. Weidenmüller, Ann. Rev. Nucl. Part. Sci. **38**, 421 (1988)
2. M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer–Verlag, Berlin, 1990); A. M. Ozorio de Almeida, *Hamiltonian Systems: Chaos and Quantization* (Cambridge University Press, Cambridge, 1990); K. Nakamura, *Quantum Chaos* (Cambridge Nonlinear Science Series, Cambridge, 1993); *From Classical to Quantum Chaos*, SIF Conference Proceedings, vol. **41**, Ed. G. F. Dell'Antonio, S. Fantoni, V. R. Manfredi (Editrice Compositori, Bologna, 1993)
3. R. U. Haq, A. Pandey, and O. Bohigas, Phys. Rev. Lett. **48**, 1086 (1982)
4. G. E. Mitchell, E. G. Bilpuch, P. M. Endt, and J. F. Jr. Shriner, Phys. Rev. Lett. **61**, 1473 (1988);
5. J. F. Jr. Shriner, E. G. Bilpuch, P. M. Endt, and G. E. Mitchell, Z. Phys. A **335**, 393 (1990); J. F. Jr. Shriner, G. E. Mitchel, and T. von Egidy, Z. Phys. A **338**, 309 (1990)
6. J. F. Jr. Shriner, G. E. Mitchell, and T. von Egidy, Z. Phys. **338**, 309 (1991)
7. J. D. Garrett, J. R. German, L. Courtney, and J. M. Espino, in *Future Directions in Nuclear Physics*, p. 345, Ed. J. Dudek and B. Haas (American Institute of Physics, New York, 1992); M. T. Lopez–Arias, V. R. Manfredi, and L. Salasnich, Riv. Nuovo Cim. **17**, N. 5, 1 (1994)
8. S. Aberg, Phys. Rev. Lett. **64**, 3119 (1990)
9. N. Whelan and Y. Alhassid, Nucl. Phys. A **556**, 42 (1993)
10. T. A. Brody, J. Flores, J. B. French, P. A. Mello, A. Pandey, and S. S. Wong, Rev. Mod. Phys. **53**, 385 (1981); H. Dias, M. S. Hussein, N. A. de Oliveira, and B. H. Wildenthal, J. Phys. G **15**, L79 (1989); V. Paar, D. Vorkapic, K. Heyde, A. G. M. van Hees, and A. A. Wolters, Phys. Lett. B **271**, 1 (1991)
11. W. E. Ormand and R.A. Broglia, Phys. Rev. C **46**, 1710 (1992)

12. M. S. Bae, T. Otshka, T. Mizusuki, and N. Fukumishi, Phys. Rev. Lett. **69**, 2349 (1992)
13. R. D. Lawson, *Theory of the Nuclear Shell Model* (Clarendon, Oxford 1980)
14. E. Caurier, computer code ANTOINE, CRN, Strasburg (1989); E. Caurier, A. P. Zuker, and A. Poves: in *Nuclear Structure of Light Nuclei far from Stability. Experiment ad Theory*, Proceedings of the Workshop, Obrnai, Ed. G. Klotz (CRN, Strasburg, 1989)
15. E. Caurier, A. P. Zuker, A. Poves, and G. Martinez–Pinedo, Phys. Rev. C **50**, 225 (1994)
16. F. J. Dyson and M. L. Mehta, J. Math. Phys. **4**, 701 (1963)
17. O. Bohigas and M. J. Giannoni, Ann. Phys. (N.Y.) **89**, 393 (1975)
18. T. A. Brody, Lett. Nuovo Cimento **7**, 482 (1973)
19. S. Raman et al., Phys. Rev. C **43**, 521 (1991)